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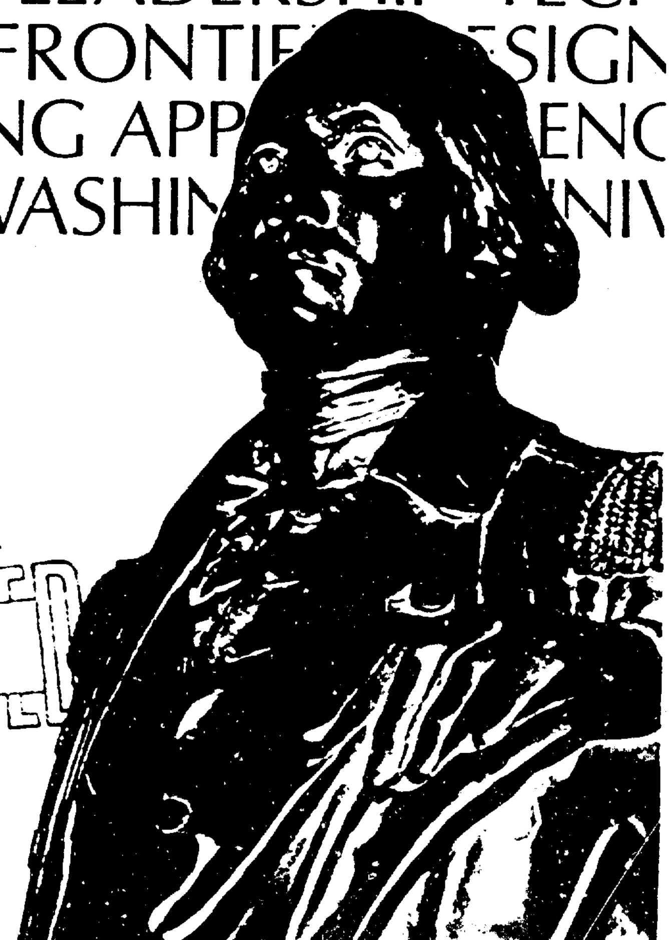

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23

ALGORITHMIC AND COMPUTATIONAL ASPECTS OF THE USE OF OPTIMIZATION METHODS IN ENGINEERING DESIGN

by

Garth P. McCormick

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1. Introduction

Since the second world war, spurred by the development and availability of computers there has been an increased effort directed toward developing methodology for solving optimization problems. Problems for solution have originated from two groups. The first, composed of economists, operations research analysts, management scientists, and planners has been concerned with the problem of how best to allocate scarce resources. Since the functional relationships in this area are not known, this group has, in the main, been content to develop programming models having only linear relationships. The success of computer codes implementing versions of the Simplex method for solving linear programming problems has reinforced the basic orientation of this group.

The second group, with a longer history, is composed of physicists, chemists, engineers, and other scientists. The problems of interest to this group contain functional relationships which, because of physical laws, are exact, and which contain nonlinear effects. Engineering optimization problems are usually ones of design. Although much thought and time has been put into the geometric and algebraic descriptions of these problems, little has been done in a systematic way to attack these problems using recent algorithmic and computational advances in nonlinear programming.

It is the intent of this paper to show how this might be done.

2. Sensitivity Analysis

Rarely is a person with a design model interested in the solution to one optimization problem. Of equal interest usually are changes in the optimal design which obtain when various aspects of the model are altered. One way to obtain this information is to solve many optimization problems containing systematic variations of the input parameters of the model and observe the changes in design.

Another way, based on recent developments in the theory characterizing a solution to an optimization problem is to use information available at the solution to a particular problem and generate a matrix which can be used independently to assess all the design changes effected by small simultaneous input parameter changes. The theory of this approach is contained in [3, Section 2.4]. The practial use of this approach is demonstrated by the following example taken from Pascual [7, p. 24], and Johnson [4, pp. 290-291].

Example 1 [Optimal Design of a Cylindrical Torsion Bar]

The problem is to find the diameter (d) and the length (L) of a cylindrical torsion bar which will transmit a virtually constant twisting torque (T), have a specified torsional rigidity (k), and for which the weight of the bar will be minimal over all those having these properties.

The mathematical programming problem is

$$\underset{(d,L)}{\text{minimize}}\ W = w\pi d^2 L/4 \tag{1}$$

subject to the constraints

$$16T/\pi d^3 \le S_t/2N\ , \tag{2}$$

$$k = \pi d^4 G/32L\ . \tag{3}$$

Here

W = weight of the torsion bar,

d = diameter of the torsion bar,

L = length of the torsion bar,

w = specific weight of the torsion bar,

G = modulus of elasticity in shear (or modulus of rigidity),

S_t = published yield strength of the material,

N = given factor of safety based on the occurrence of yielding as the failure phenomenon,

T = the torque, and

k = the prescribed torsional rigidity.

The expression for weight in (1) is simply the volume of the cylindrical torsion bar times the specific density. The expression on the left of (2) gives the maximum state of shear stress experienced by the bar for the applied torque T. This occurs at the outer edge of the bar and is the same along its length. This must not exceed the experimentally determined yield point of the bar or permanent distortion will result. Equation (3) gives the torsional rigidity which is a function of the diameter of the bar as well as its modulus of rigidity. The higher the k value the less temporary deformation is experienced by the bar when torque is applied to it.

For this model, values of the parameters used were $w = 490$ lbs/ft^3, $G = 11.5 \times 10^6$ psi, $S_t = 35{,}000$ psi, $N = 2$, $T = 1000$ lb-in, and $k = 10^5$ lb-in.

For purposes of convenience the problem is rewritten

$$\underset{(d,L)}{\text{minimize}} \quad w\pi d^2 L/4$$

$$\text{subject to} \quad \pi d^3 S_t - 32NT \geq 0 \,, \tag{4}$$

$$32Lk - \pi d^4 G = 0 \,. \tag{5}$$

The solution to this problem occurs at $(d^*,L^*) = (.834937, 5.486689)$, (both quantities in inches). The generalized Lagrange multiplier associated with the inequality constraint is $u_1^* = .186342 \times 10^{-2}$, and the Lagrange multiplier associated with the equality constraint has a value $w_1^* = .485175 \times 10^{-6}$. These are the values for which the gradient of the Lagrangian function

$$\mathcal{L}(d,L,u_1,w_1) = w\pi d^2L/4 - u_1(\pi d^3S_t - 32NT) + w_1(32Lk - \pi d^4G)$$

vanishes, i.e., for which

$$\begin{bmatrix} w\pi dL/2 \\ w\pi d^2/4 \end{bmatrix} - \begin{bmatrix} 3\pi d^2S_t \\ 0 \end{bmatrix} u_1 + \begin{bmatrix} -4\pi d^3G \\ 32k \end{bmatrix} w_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

The interpretation of the Lagrange multiplier is well-known. If the right hand side of (4) is changed to δ, then the solution to the perturbed problem has an optimal objective function value which differs from that of the problem just solved by approximately δu_1^*. What is not so well-known is that information is available to answer the question of how the minimizing point itself changes when general perturbations are placed on the above problem.

To illustrate this without giving the general formulation which is contained in [3, section 2.4], suppose the question was posed for the above example how much would the solution change if the torsional rigidity requirement (k) were changed from 100,000 lb-in to 102,000 lb-in and simultaneously the torque (T) from 1000 lb-in to 1030.301 lb-in ?

From the general theory in [3] we obtain the result that the problem resulting from the replacement in (4) of T by $T + \Delta T$, and in (5) k by $k + \Delta k$ results in a new minimizing vector and associated Lagrange multipliers which can be approximated from those of the original problem by the expression

$$\begin{bmatrix} d^* \\ L^* \\ u_1^* \\ w_1^* \end{bmatrix} + \begin{bmatrix} w\pi L/2-6\pi d^* S_t u_1^* - 12(d^*)^2 G w_1^*, & w\pi d^*/2, & -3\pi(d^*)^2 S_t, & -4\pi(d^*)^3 G \\ w\pi d^*/2 & , \ 0 & , \ 0 & , \ 32k \\ u_1^*(3\pi(d^*)^2 S_t) & , \ 0 & , \ 0 & , \ 0 \\ -4\pi(d^*)^3 G & , \ 32k & , \ 0 & , \ 0 \end{bmatrix}^{-1} \begin{bmatrix} 0, & 0 \\ 0, & 32w_1^* \\ 64u_1^*, & 0 \\ 0, & -32L^* \end{bmatrix} \begin{bmatrix} \Delta T \\ \Delta k \end{bmatrix}.$$

Using $\Delta T = 30.301$, and $\Delta k = 2{,}000$, computation of the above quantities yields the expected change in the optimal d and L as (.00843,.11193) . For comparison purposes, the perturbed problem has a solution which differs from the original one by (.00834,.11083).. Thus the approximation agrees with the exact change to about 3 significant figures.

In some problems it is not a priori obvious even the direction of change of the problem solution when the values of many parameters are changed simultaneously. The use of sensitivity information should have wide application in the area of engineering design.

3. Obtaining Global as Opposed to Local Solutions by Use of Branch and Bound Techniques

Most algorithms for solving nonlinear programming problems are only guaranteed to find global (as opposed to local) solutions when the problem functions describe a convex programming problem. Problems which can trap an algorithm at a local solution often arise when the objective function (to be minimized) is a total cost function with decreasing marginal costs. A simple picture is contained in Figure 1. The curve shown in Figure 1 is concave whereas if it were convex, its use in an optimization problem would cause no difficulty. To illustrate the difficulties this can cause and also to illustrate the increasingly important branch and bound approach for solving these problems we consider the following example. It is taken from the area of water pollution control which is becoming a source of optimization problems which involve both groups of people, the social and physical scientists mentioned in the introduction.

Example 2 [Optimal Reservoir Design]

The concentration of dissolved oxygen in the water of a certain section of a river is below the acceptable level due to pollution of the river. It is desired to increase the level of dissolved oxygen to the acceptable level by building reservoirs at one or more upstream points of the river so as to be able to augment the river flow and dilute the wastes.

Although the original model contained many sites, for illustrative pusposes we consider an idealized model with two sites. Let x_j be the flow augmentation at site j, $j = 1,2$, and $1x_1^{.25}$ be the cost to build a reservoir at site 1 to augment the flow by amount x_1, and let $2x_2^{.25}$ be the cost to

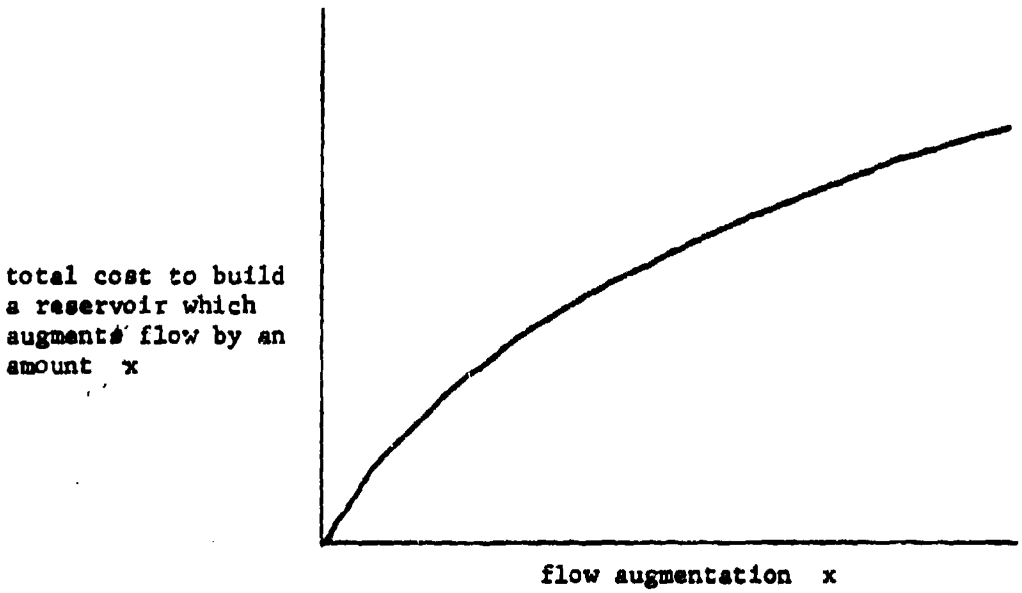

Figure 1. A Concave Function of One Variable

build a reservoir at site 2 to augment the flow by amount x_2. Assume that the required augmentation is 3. Algebraically stated then the optimization problem is to find x_1^* and x_2^* which minimize the total cost

$$1x_1^{.5} + 2x_2^{.25}$$

subject to the constraints

$$x_1 + x_2 \geq 3,\ x_1 \geq 0,\ x_2 \geq 0,\ x_1 \leq 6,\ x_2 \leq 5 .$$

The region of feasible points along with two curves of constant costs are plotted in Figure 2.

It is obvious that (0,3) and (3,0) are local solutions to the problem, i.e., that in a region about either point all information indicates that that point is a solution. Just about any algorithm which tries to solve this problem will go to either solution depending upon the initial starting point. A guarantee of the ability of an algorithm to obtain a global (as opposed to local) solution is required.

Recently branch and bound methodology [1], [9] has been applied to problems of the above form in order to guarantee convergence to a global solution. Rather than define what a branch and bound method is in general, the problem just stated will be solved by such an algorithm.

The basic branch and bound approach for solving the nonconvex programming problem is to solve a sequence of underestimating convex programming problems which apply to subregions of the feasible region. A sequence of underestimating values for the solution of the original problem is created which approaches the optimal value from below. First a convex (in this case linear) underestimate is generated of the objective function in the rectangle $0 \leq x_1 \leq 6,\ 0 \leq x_2 \leq 5$. Figures 3 and 4 show that the linear function $.408x_1$ is a linear underestimate of the function $x_1^{.5}$ in the interval

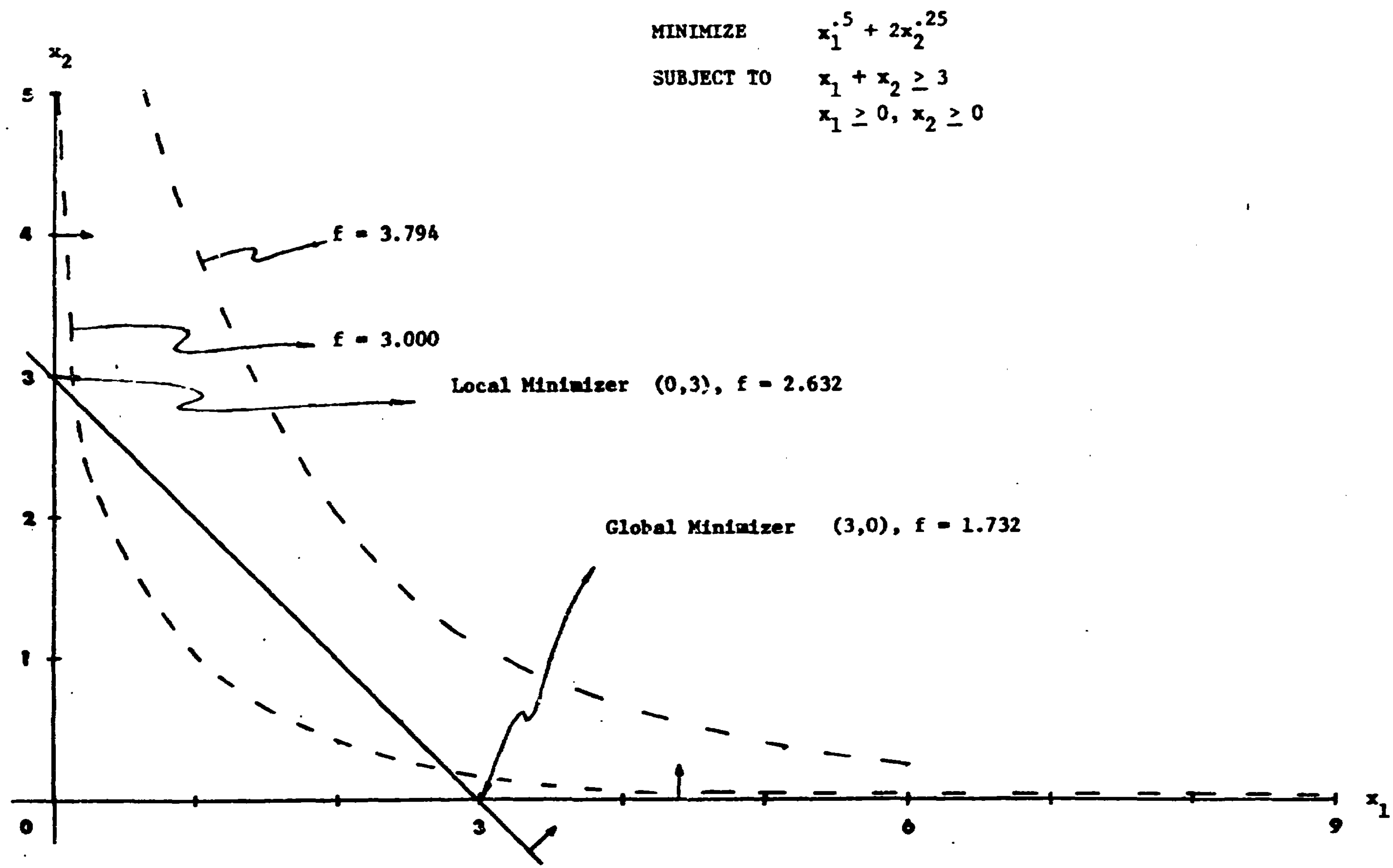

Figure 2. Optimization Problem with Two Local Minimizers

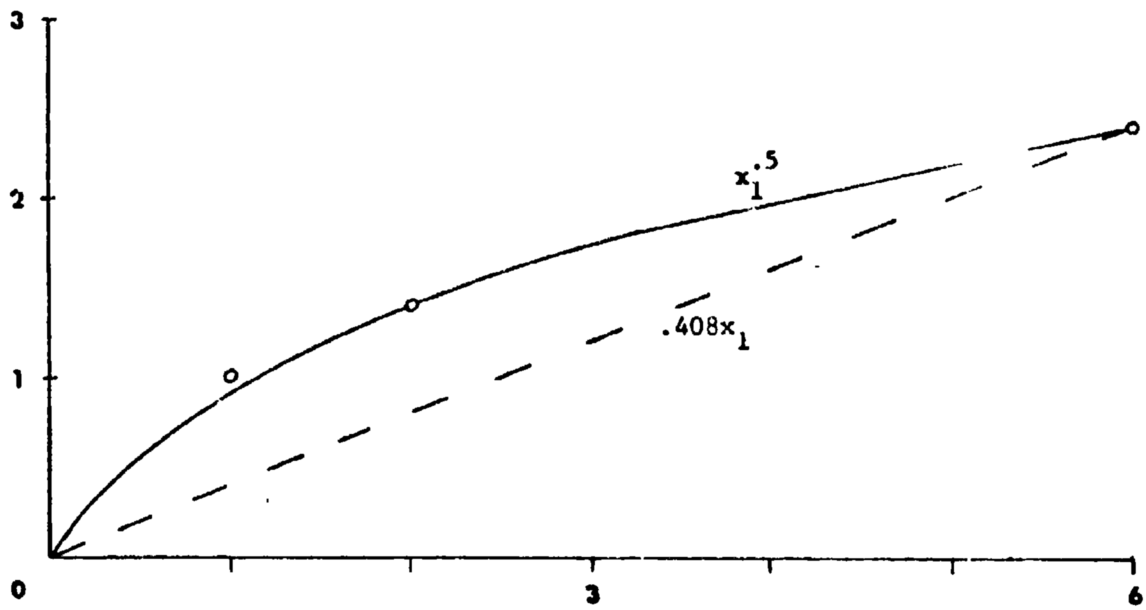

Figure 3. Concave Function of x_1 with Underestimating Convex Envelope

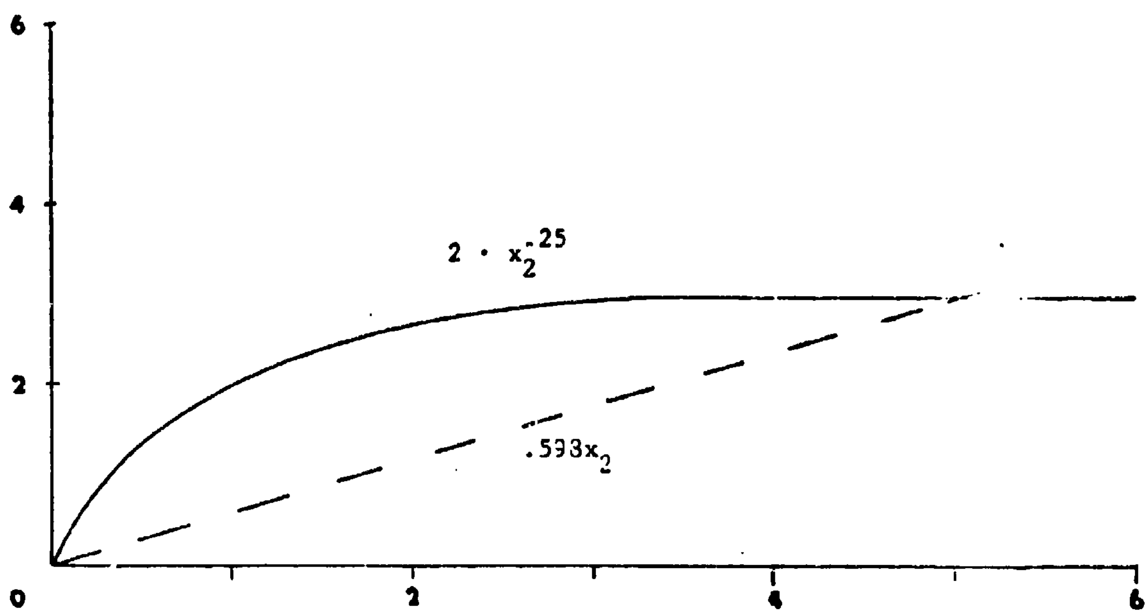

Figure 4. Concave Function of x_2 with Underestimating Convex Envelope

$[0,6]$, and that $.598x_2$ is a linear underestimate of $2x_2^{.25}$ in the interval $[0,5]$. In fact these straight lines are the highest convex functions which underestimate the original ones in those intervals.

The following programming problem is an underestimating convex (linear in this case) programming problem for the original nonconvex one. Find values of x_1 and x_2 which

$$\text{minimize } .408x_1 + .598x_2$$

subject to the constraints

$$x_1 + x_2 \geq 3,\ 0 \leq x_1 \leq 6,\ 0 \leq x_2 \leq 5 .$$

The solution to this problem is at $x^* = (3,0)$, with an objective function value (of the linear underestimating function) of 1.224. Thus we know that the global minimizing value to the original problem is bounded below by 1.224.

The next step in the procedure is to divide the original rectangle into two parts and solve an underestimating problem for each part which is 'closer to' the original problem than the first underestimating problem solved above. The decision on how to divide is made by choosing that variable for which the difference in function values between the underestimating function and the original function is greatest. Using this criterion, the decision is made to split the original rectangle into two parts on x_1 , yielding the new sets of constraints $0 \leq x_1 \leq 3,\ 0 \leq x_2 \leq 5$, and $3 \leq x_1 \leq 6,\ 0 \leq x_2 \leq 5$. Using the same approach for generating convex underestimating envelopes the first new programming problem to be solved is

$$\text{minimize } .577x_1 + .598x_2$$

$$\text{subject to } 0 \leq x_1 \leq 3,\ 0 \leq x_2 \leq 5,\ x_1 + x_2 \geq 3$$

which has a solution at (3,0) with solution value 1.732.

The problem associated with the other rectangle is

$$\text{minimize} \quad 1.015 + .239x_1 + .598x_2$$

$$\text{subject to} \quad 3 \leq x_1 \leq 6,\ 0 \leq x_2 \leq 5,\ x_1 + x_2 \geq 3$$

which has a solution at (3,0) with solution value 1.732 also. Since both values are lower bounds to the global optimum, and since $(3)^{.5} + 2(0)^{.25} = 1.732$, the global solution has been obtained.

Branch and bound techniques can also be used to handle problems which are not well-behaved in that the functions lack the proper smoothness or continuity properties. Also, these techniques to date are the most successful approaches for solving combinatorial problems, e.g., problems where the difficulty is in ascertaining the <u>order</u> in which activities are to be performed, or <u>whether</u> <u>or</u> <u>not</u> to perform them rather than the optimal <u>level</u> of any activity.

4. Computer Code-Optimization Model Interface

A major hurdle to the computer solution of nonlinear optimization problems in engineering design is the lack of an automated procedure for giving codes all the inputs an algorithm needs to solve the problem. For example, the branch and bound procedure applied to the problem in the previous section is general enough to solve separable programming problems of the form

$$\text{minimize} \quad \Sigma_{j=1}^{n} f_j(x_j)$$

$$\text{subject to} \quad \Sigma_{j=1}^{n} g_{ij}(x_j) \geq 0, \; i = 1,\ldots,m \; .$$

A further requirement is that for any function, say $f_j(x_j)$ in any given interval $[L_j, U_j]$, the user must supply a function $d_j(x_j)$ which is the convex envelope of $f_j(x_j)$ in the interval. That is, one must supply to the computer code implementing the branch and bound method the highest convex envelope which underestimates the function $f_j(x_j)$ in that interval.

For another example, the code implementing the sequential unconstrained minimization technique (SUMT) [5], [3] requires the user to supply the first derivatives of the problem functions. To be efficient, the code asks the user to supply the second derivatives. A certain amount of this trouble can be avoided by the use of difference approximations instead of the analytic forms, but it is no wonder that engineers in the design area are more inclined to use heuristically based algorithms such as the SIMPLEX SEARCH method [6] for solving their optimization problems which require only function values.

One solution to this problem has been the development of a language [8] and a computer program which automatically computes first and second derivatives of an algebraic expression when the problem functions are written down in the language by the user. In (6) is an expression giving the first stage

velocity of a three stage space launch vehicle as a function of design variables written in this language. The FORTRAN-like expression is

$$X(14)*T1*GBAR*LØG(1./X(13))/X(15) \quad . \tag{6}$$

where

X(14) = stage 1 total thrust in thousands of pounds,

T1 = stage 1 burn time in seconds,

X(13) = stage 1 mass fraction (dimensionless),

GBAR = gravity constant, and

LØG = natural logarithm function.

The first four quantities above are design variables of the optimization model [1, Chapter 2], which was to produce a minimum cost design satisfying certain performance characteristics. Its solution using SUMT required the supplying of a computer program for the analytic derivatives of expressions like the one in (6). This was an extremely time consuming and an error prone enterprise. Using the new language, such model implementation is much more feasible.

Another approach to this problem now under consideration is to first convert the programming problem into a separable problem and devise a card format for separable terms allowing for any conveivable functions of a single variable. Computer routines could be coded and used to compute the derivatives, first and second, and the convex envelopes of functions of a single variable.

The general procedure for converting an optimization problem to a separable problem is to add variables and increase the number of constraints. As an example, consider the following which expresses the requirement that the section modulus of a vertical transverse corrugated bulkhead satisfy certain rules contained in Det Norske Veritas. The inequality is [1, p. 56],

$$\frac{1}{6} x_2 x_3 x_4 + \frac{a}{2} x_1 x_3 x_4 - kh_t \ell_t^2 [x_1 + (x_2^2 - x_3^2)^{1/2}] \geq 0 .$$

This constraint can be 'separated' by the addition of three more variables and three constraints. The resulting constraints are

$$\ln x_3 + \ln x_4 + x_5 - \ln(kh_t \ell_t^2) - \ln x_4 \geq 0 ,$$

$$x_1 + x_6 = x_4$$

$$\frac{1}{6} x_2 + \frac{a}{2} x_1 = e^{x_5}$$

$$x_2^2 - x_3^2 = x_6^2 .$$

A computer code can probably be developed to take the functions written in the language described in [8] and do the conversions required to separate the problem.

5. Conclusion

In this paper, a brief summary of some recent powerful theoretical tools for sensitivity analysis in engineering design, and recent globally convergent algorithms for solving optimization problems have been given. The barrier to using these tools and other recent algorithms for solving problems is the lack of a readily available, easily used language in which to describe the optimization models. The language developed by Pugh [8] is a step toward eliminating this barrier. Future progress will depend in large part on bringing together those with the algorithmic ability, those with the design optimization problems, and those with the capability of developing computer systems.

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